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Dynamics of Bose-Einstein Condensates with Long-Range Attractive Interactions

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We solve the time-dependent Gross-Pitaevskii equation for the Bose-Einstein condensate with non-local dipole-dipole interaction potential as well as with the attractive gravity-like potential numerically. We observe formation of supersolid structure above the critical intensity in harmonic traps. Simple Linear Combination of Gaussian Orbitals (LCGO) theory is provided. We also observe self-bound structures for the condensate with gravity-like potentials.

1 Introduction

The laboratory observation of Bose-Einstein condensates created from cold atoms[1] opened new opportunities for theoretical investigation of those fascinating systems. The old Gross-Pitaevskii equation[2], probably the most beautiful example of the density functional theory[3,4], became rediscovered to provide information both about the condensate equilibrium density as well as dynamical properties[5,6]. New variation of possibilities emerged from novel experimental techniques either known or impossible for the condensed matter experiments. These were the observation of elementary excitations[7], wave matter lasing effect[9,10], as well as solid state modeling and control in optical lattices[11,12]. Quite recently new proposals of inducing variety of interactions much more complicated then simply hard-ball collisional one have been formulated[13–15]. The combination of few laser beams was shown to generate an attractive long-range interactions within the Bose-Einstein condestate due to the interplay between dipole-dipole forces[14]. This was equivalent to the gravity forces with enormously large modeled gravitational constant. The quantum phase transition of the density modulation[16] by the dipole-dipole optical interaction has been predicted from the variational calculations[17]. The question rose if it is the artificial effect of the variational methods.

In the following we show the existence of supersolid ground states by the direct integration of the Gross-Pitaevskii (G-P) equation using the imaginary time integration method in 3 spatial dimensions and without any prior assumption on the symmetry of the condensate. Non-dispersing structures of the condensate are also observed numerically without the external trap for soft-core model potentials.

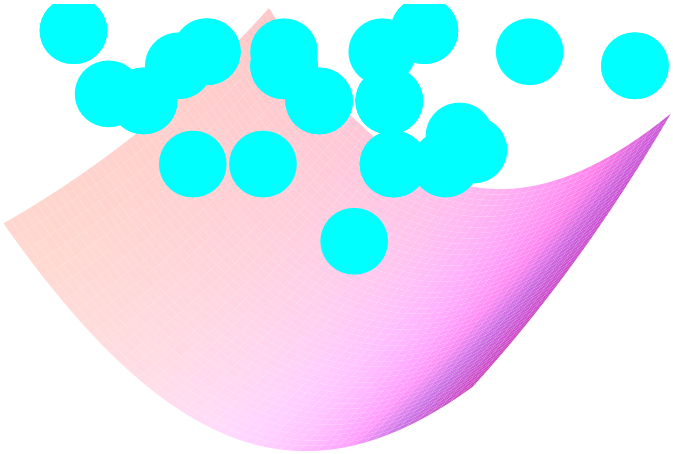

Figure 1. Classical picture of the Bose-Einstein condensate in the trap. All atoms try to occupy the same quantum state described by the mean field ψ.

2 Gross-Pitaevskii Equation

We start our analysis from the time dependent G-P equation[2] for the Bose-Condensate with nonlocal inter-particle interaction. The Hamiltonian of our system can be written in the second quantization form as

$$\hat{H} = -\int \Psi^\dagger(\mathbf{x})[\triangle/2 - V(\mathbf{x})]\Psi(\mathbf{x}) + \alpha \int \Psi^\dagger(\mathbf{x})\Psi^\dagger(\mathbf{x})\Psi(\mathbf{x})\Psi(\mathbf{x}) + \gamma \int\int \Psi^\dagger(\mathbf{x})\Psi^\dagger(\mathbf{x})V_{dd}(\mathbf{x}-\mathbf{y})\Psi(\mathbf{y})\Psi(\mathbf{y}), \quad (1)$$

where we use the dipole-dipole induced potential generated by circularly polarized external field

$$V_{dd} = \gamma\Big[\frac{2z^2 - x^2 - y^2}{r^5}(\cos(r) + r\sin(r)) - \frac{2z^2 + x^2 + y^2}{r^3}\cos(r)\Big]\cos(z). \quad (2)$$

Here $\Psi^\dagger, \Psi$ are the bosonic field operators obeying the standard commutation relations in space

$$[\Psi(\mathbf{x}), \Psi^\dagger(\mathbf{y})] = \delta(\mathbf{x}-\mathbf{y}). \quad (3)$$

One can obtain the mean-field equation by neglecting the following correlations

$$< \Psi^\dagger(\mathbf{x})\Psi^\dagger(\mathbf{x})\Psi(\mathbf{x})\Psi(\mathbf{x}) > \approx \rho(\mathbf{x})^2 \quad (4)$$

with the density of the condensate

$$\rho(\mathbf{x}) = < \Psi^\dagger(\mathbf{x})\Psi(\mathbf{x}) > = \psi(\mathbf{x})^*\psi(\mathbf{x}). \quad (5)$$

It justifies the time-dependent G-P equation as obtained within the density functional theory[4] from the variational principle

$$\frac{\delta < H - id/dt >}{\delta \rho} = 0. \tag{6}$$

This yields the following G-P equation

$$-[\triangle/2 + V(\mathbf{x}) + \alpha|\psi(\mathbf{x}t)|^2]\psi(\mathbf{x}t) + \gamma \int \rho(\mathbf{y}t) V_{dd}(\mathbf{x}-\mathbf{y})\psi(\mathbf{x}t) = i\frac{d\psi(\mathbf{x}t)}{dt}. \tag{7}$$

3 Supersolids

To predict the supersolid formation it is enough to notice that the potential V_{dd} is quasi-periodic (Fig. 1). One expects the solid formation for the minima which are deep enough according to the modified Bloch theory. The periodic part of the Bloch function now becomes quasi-periodic

$$\psi_k = e^{ik\mathbf{x}} u(\mathbf{x}) \quad u(\mathbf{x}) \approx u(\mathbf{x} + \pi n). \tag{8}$$

In the analogy to the Linear Combination of Atomic Orbitals, the Bloch function can be written as the Linear Combination of Gaussian Orbitals (LCGO) with originally unspecified widths, namely

$$\psi_0(\mathbf{x}) = \sum e^{ikz_n} \phi_n(\mathbf{x} - z_n) \tag{9}$$

and so the ground state for $k = 0$. Note that the Gaussian orbitals are now different in the contrast to classic LCAO method due to predicted deviation from the perfect translational symmetry

$$\phi_n(\mathbf{x}) = C_n e^{-a_n^2(x^2+y^2)/2} e^{-b_n^2(z-z_n)^2/2}. \tag{10}$$

Further we make the zero nearest-neighbors approximation for the condensate density by keeping only the self overlap

$$\rho(\mathbf{x}) = \sum |\phi_n(\mathbf{x} - z_n)|^2. \tag{11}$$

We obtain the following system of equations

$$\begin{aligned}[-\frac{\triangle}{2} + V(\mathbf{x}) + \alpha\rho(\mathbf{x})]\phi_i(\mathbf{x} - z_i) + \sum \int V_{dd}(\mathbf{x}-\mathbf{y})|\phi_n(\mathbf{x} - z_n)|^2 \phi_i(\mathbf{x} - z_i) \\ = E\phi_i(\mathbf{x} - z_i).\end{aligned} \tag{12}$$

We assume the harmonic trap potential, which is prolate and cylindrically symmetric

$$V(\mathbf{x}) = \frac{1}{2}\omega_r^2(x^2 + y^2) + \frac{1}{2}\omega_z z^2 \tag{13}$$

and more

$$\begin{aligned}\int V_{dd}(\mathbf{x}-\mathbf{y})|\phi_n(\mathbf{x} - z_n)|^2 \phi_n(\mathbf{x} - z_i) = \\ [\frac{1}{2}\omega_{nri}^2(x^2 + y^2) + \frac{1}{2}\omega_{nzi}(z - z_i)^2]\phi_n(\mathbf{x} - z_i),\end{aligned} \tag{14}$$

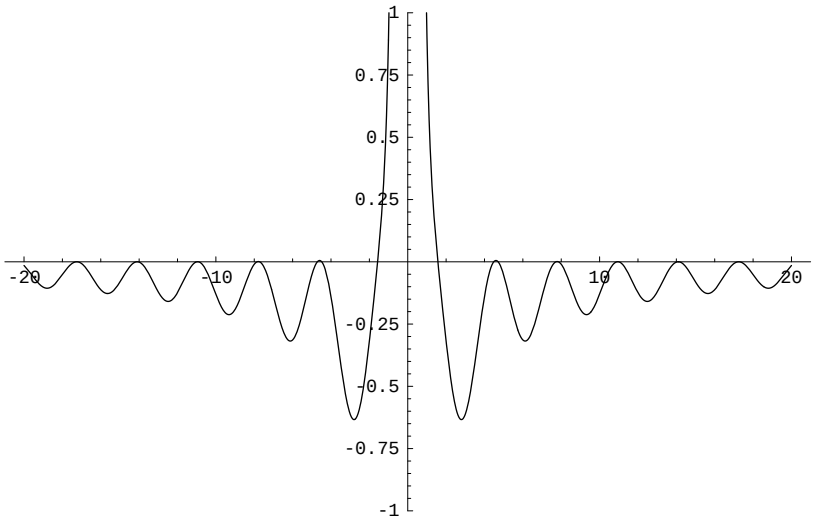

Figure 2. The dipole-dipole interaction potential on the $x = y = 0$ line. One expects the solid formation due to the quasi-periodicity.

where

$$\omega_{nri}^2 = \frac{d^2 \int V_{dd}(\mathbf{x}-\mathbf{y})|\phi_n(\mathbf{y}-z_n)|^2}{dx^2}|_{00z_i} \tag{15}$$

$$\omega_{nzi}^2 = \frac{d^2 \int V_{dd}(\mathbf{x}-\mathbf{y})|\phi_n(\mathbf{y}-z_n)|^2}{dz^2}|_{00z_i}. \tag{16}$$

Further we assume for the hard self-interaction

$$|\phi_n(\mathbf{x}-z_i)|^2 = -C_n a_n^2(x^2+y^2) - C_n b_n^2 z_i^2 \tag{17}$$

which closes the system of equation for z_i and a_n, b_z.

One expects the clear density modulation (supersolid) when the frequencies generated by the self-interaction are much larger then the longitudinal frequency of the harmonic trap

$$\Omega_{nzi}^2 = \omega_{nzi}^2 - \alpha C_n b_n^2 > \omega_z^2 \tag{18}$$

and also if there is no external confinement leading to Gaussian orbital widths narrower then the period of the the solid

$$\Omega_{nzi}^{-1/2} < \pi. \tag{19}$$

This defines constraints for the sufficiently large γ.

To obtain the simplest approximate solutions of (1-3) it is enough to assume sharp Gaussian approximation for functions ϕ_n for the purpose of calculating the dipole-dipole integrals

$$|\phi_n(\mathbf{x}-z_i)|^2 = \delta(\mathbf{x}-z_i) \tag{20}$$

or sharply picked supersolid. The minima of the corresponding superposition potential

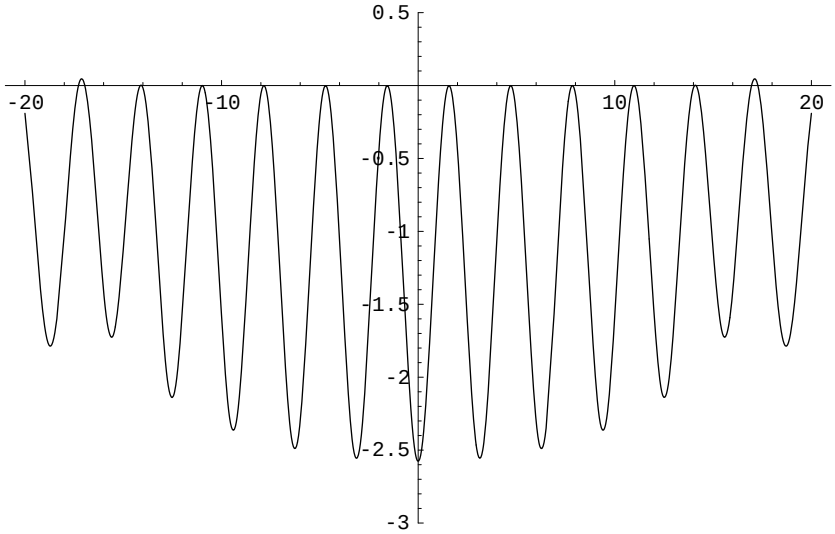

Figure 3. The potential $\sum(z)$ on the line $x = y = 0$. Note that the minima of the superposition correspond approximately to the original positions of delta-like orbitals.

$\sum(z) = \sum V_{dd}(x, y, z - i\pi)$ are the measure of self-consistency of the first iteration. For a solid consisting of 11 minima and assumed initial perfectly periodic $z_i = i\pi$ solid we obtain from summation of the potential, $z_0 = 0.0000$, $z_{\pm 1} = \pm 3.1358$, $z_{\pm 2} = \pm 6.2701$, $z_{\pm 3} = \pm 9.4001$, $z_{\pm 4} = \pm 12.5173$, and $z_{\pm 5} = 15.5874$ where we used the soft core potential further used in our numerical simulations

$$V_{dd} = \gamma\Big[\frac{2z^2 - x^2 - y^2}{r_e^5}(\cos(r) + r\sin(r)) - \frac{2z^2 + x^2 + y^2}{r_e^3}\cos(r)\Big]\cos(z) \quad (21)$$

with "soft" r_e

$$r_e = \sqrt{x^2 + y^2 + z^2 + 1}. \quad (22)$$

Therefore the solid is self-sustained when the density distribution generates components of the interaction potential shifted by the lattice constant of the solid.

4 Self-Binding of the Condensate

Consider a more general form of the dipole-dipole interaction potential between atoms of the condensate induced by the external laser field with the intensity I

$$U(\mathbf{r}) = \frac{I}{4\pi c\epsilon_0^2}\alpha^2(q)\mathbf{e}_i\mathbf{e}_i^* V_{ij}(q, \mathbf{r})\cos(\mathbf{q}\cdot\mathbf{r}) \quad (23)$$

$$V_{ij} = \frac{1}{r^3}[(\delta_{ij} - 3\mathbf{r}_i\mathbf{r}_j)(\cos qr + qr\sin qr) - (\delta_{ij} - \mathbf{r}_i\mathbf{r}_j)q^2r^2\cos qr].$$

The three-beam potential resulted from the circular polarization of orthogonal beams simplifies to

$$U(\mathbf{r}) = -\frac{3Iq^2\alpha^2}{16\pi c\epsilon_0^2}\frac{1}{r}\Big[\frac{7}{3} + (\sin\theta\cos\phi)^4 + (\sin\theta\sin\phi)^4 + (\cos\theta)^4\Big]. \tag{24}$$

Finally, 18 beams can be superposed to achieve total cancelation of angular factors, namely

$$U(\mathbf{r}) = -\frac{11}{4\pi}\frac{Iq^2\alpha^2}{c\epsilon_0^2}\frac{1}{r} = -\frac{u}{r}. \tag{25}$$

Note that this is effectively gravitational-like potential with an enormously large gravity constant.

The existence of non-dispersing, self-bound structures of the condensate density can be predicted from two simple approximations. First, one may use the sharp density approximation for the purpose of self-interaction integral in the stationary G-P equation

$$[-\triangle/2 + V(\mathbf{x}) + \alpha|\psi(\mathbf{x})|^2]\psi(\mathbf{x}) + \int \rho(\mathbf{y})V_{dd}(\mathbf{x}-\mathbf{y})\psi(\mathbf{x}t) = E\psi(\mathbf{x}) \tag{26}$$

where now

$$V_{dd}(\mathbf{x}-\mathbf{y}) = -\frac{u}{|\mathbf{x}-\mathbf{y}|}. \tag{27}$$

This can be done by assuming

$$|\psi(\mathbf{x})|^2 = \delta(\mathbf{x}). \tag{28}$$

The equation (26) (we assumed $\alpha = 0$ for simplicity) has now a simple solution since it also describes the stationary atom of Hydrogen

$$\psi(\mathbf{x}) = Ce^{-u\sqrt{(x^2+y^2+z^2)}}. \tag{29}$$

This is self-bound non-dispersing condensate density with exponential profile.

Alternatively, one can assume the Gaussian condensate profile

$$\psi(\mathbf{x}) = Ce^{-a^2(x^2+y^2+z^2)/2} \tag{30}$$

and seek the harmonic approximation for the self-interaction

$$\int V_{dd}(\mathbf{x}-\mathbf{y})|\psi(\mathbf{y})|^2\psi(\mathbf{x}) = \frac{1}{2}\omega^2(x^2+y^2+z^2)\psi(\mathbf{x}) \tag{31}$$

where

$$\omega^2 = \frac{d^2\int V_{dd}(\mathbf{x}-\mathbf{y})|\psi(\mathbf{y})|^2}{dx^2}|_{000} \tag{32}$$

and further for the hard self-interaction ($\alpha \neq 0$)

$$|\psi_n(\mathbf{x})|^2 = -Ca^2(x^2+y^2+z^2) \tag{33}$$

which closes the system of equations for ω and a. Therefore Gaussian self-bound condensate density is predicted from the second approach.

Obviously the true ground state which is expected to be between the Gaussian and exponential can be obtained and confirmed only numerically.

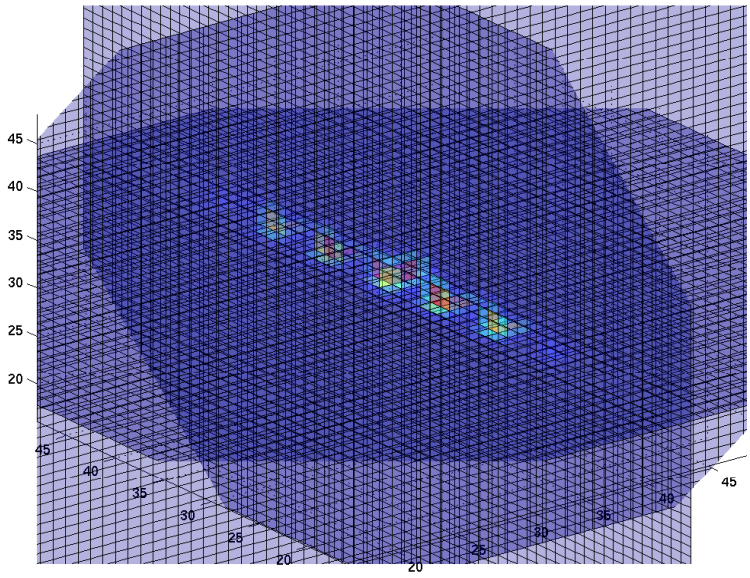

Figure 4. Volumetric plot of supersolid formed during imaginary time integration. The peaks of the condensate density are separated approximately by π.

5 Numerical Solutions

In order to check our predictions numerically we have solved the Gross-Pitaevskii equation using the imaginary integration time method[21]. For the density dependent hamiltonian H one can assume the existence of the instantaneous spectrum ϵ_i at the certain time $t = i\tau$

$$H[\rho, t]\psi_i = \epsilon_i \psi_i. \tag{34}$$

Thus in the series representing the infinitesimal solution

$$\psi(0 + \delta t) = c_0\psi_0 e^{\epsilon_0 \delta\tau} + ... + c_n\psi_n e^{\epsilon_n \delta\tau} \tag{35}$$

only the term with the lowest instantaneous energy ϵ_0 is magnified and the procedure leads to finding the ground state of the system. For the Gross-Pitaevskii propagator we used the second order split operator method[22,23]. The nonlinear propagator was approximated as follows

$$e^{-i\int H(t)dt} \approx e^{-iV[\rho]dt/2} e^{-iTdt} e^{-iV[\rho]dt/2} \tag{36}$$

with

$$V[\rho] = \frac{1}{2}\omega_r^2(x^2 + y^2) + \frac{1}{2}\omega_z^2 z^2 + \alpha\rho(\mathbf{x}t) + \gamma \int V_{dd}(\mathbf{x} - \mathbf{y})\rho(\mathbf{y}t) \tag{37}$$

and the kinetic energy part calculated with Fast Fourier Transform $\mathcal{F}_k$

$$e^{-iTdt} = \mathcal{F}_k^{-1} e^{-k^2 dt/2} \mathcal{F}_k. \tag{38}$$

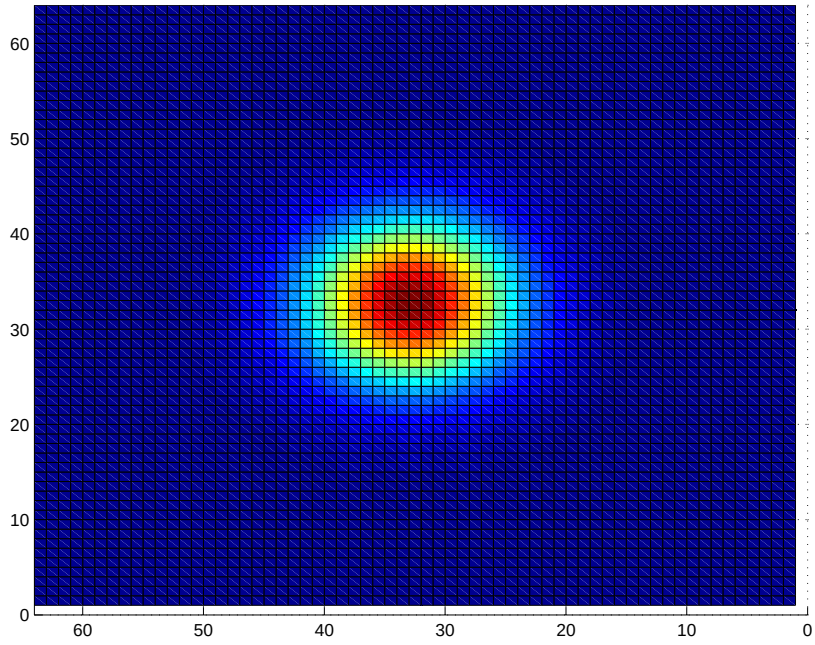

Figure 5. Volumetric plot of self-bound condensate formed during imaginary time integration for $u = 1.0$. The distribution will stably oscillate if perturbed from the equilibrium.

The essential problem for this kind of nonlocal equation is the fast calculation of the nonlocal part of the potential $V[\rho]$. We again used the Fast Fourier Transform to calculate the convolution

$$\int V_{dd}(\mathbf{x}-\mathbf{y})\rho(\mathbf{y}) = \mathcal{F}_k^{-1}[\rho(\mathbf{k})V_{dd}(\mathbf{k})]. \tag{39}$$

In our calculations we used the soft-core dipole-dipole potential (16) with its Coulomb version $1/\sqrt{x^2+1}$ widely used in the one dimensional strong field physics[24]. This allowed us to observe supersolids without the hard core repulsion ($\alpha = 0$), otherwise leading to collapse of the condensate and is somehow similar to introducing hard-ball repulsion to stabilize the system[17] The initial state was chosen to be a Gaussian ground state of the harmonic oscillator of the atom trap

$$\phi(\mathbf{x}0) = Ce^{-\omega_r(x^2+y^2)/2-\omega_z z^2/2} \tag{40}$$

to cover many wavelengths of the self-interaction potential. Fig. 4 shows the volumetric plot of the condensate density for the value of the coupling constat γ sufficient to create the supersolid. We see clear density modulation in the longitudinal direction of the condensate. The separation of peaks is approximately by π in units of qz as predicted by simple theory. Fig. 5 shows the condensate density obtained from the simulations with gravity-like potential. The self-bound, stable structure is formed during the imaginary-time evolution.

6 Conclusions

Supercomputer simulation is the powerful tool for studies of Bose-Einstein condensates with interactions. The Schrödinger equation for N bosons is still impossible to solve numerically, however mean-field Gross-Pitaevskii theory is feasible for the numerical treatment in three dimensions. Using this technique we have observed transition to supersolid density modulation in Bose-Einstein condensate using the imaginary time split-operator method. The simulations were free from the variational constraints. We have also observed self-binding of the condensate with modeled gravitational attraction.

Acknowledgments

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